An Azobenzene Photoswitch Sheds Light on Turn Nucleation in Amyloid-β Self-Assembly

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ELECTRONIC SUPPORTING INFORMATION

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Figure S1. Analytical HPLC trace (215 nm) of *trans*-**2** to *cis*-**2** conversion in water. The peak at 12.1 min is *cis*-**2** and the peak at 12.2 minutes is residual *trans*-**2**.

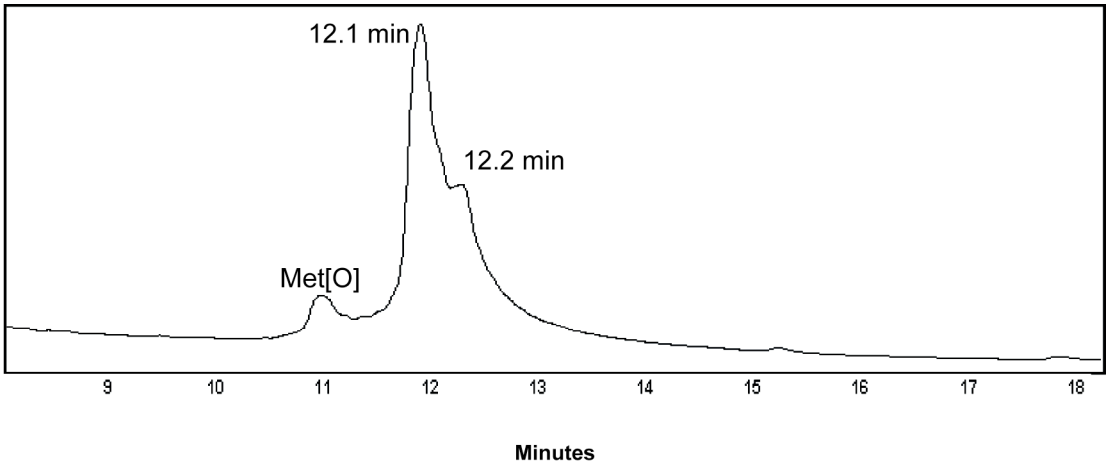

Figure S2. Analytical HPLC trace (215 nm) of *trans*-**3** to *cis*-**3** conversion in water. The peak at 11.9 minutes is *cis*-**3** and the peak at 12.3 minutes is residual *trans*-**3**.

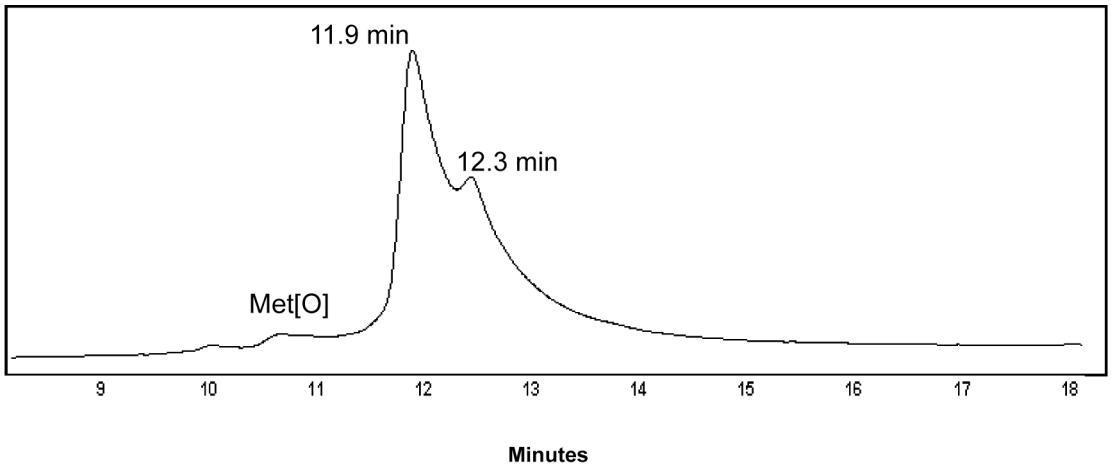

Figure S3. Digital images of aggregate pellets from peptides **1** and *trans*-**2** and *cis*-**2** after Congo red staining

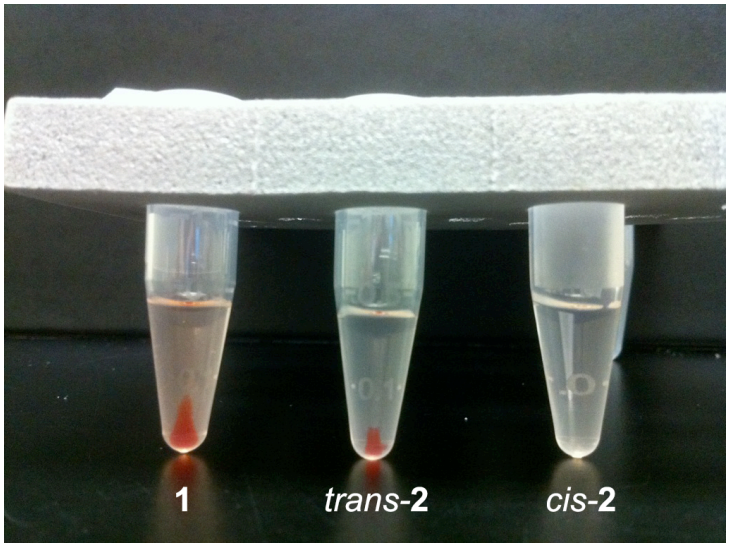

Figure S4. A. Congo red absorbance spectra in the presence and absence of *trans*-**2** and *cis*-**2**. B. Congo red absorbance spectra for *trans*-**2** and *cis*-**2** with the spectrum for Congo red alone removed.

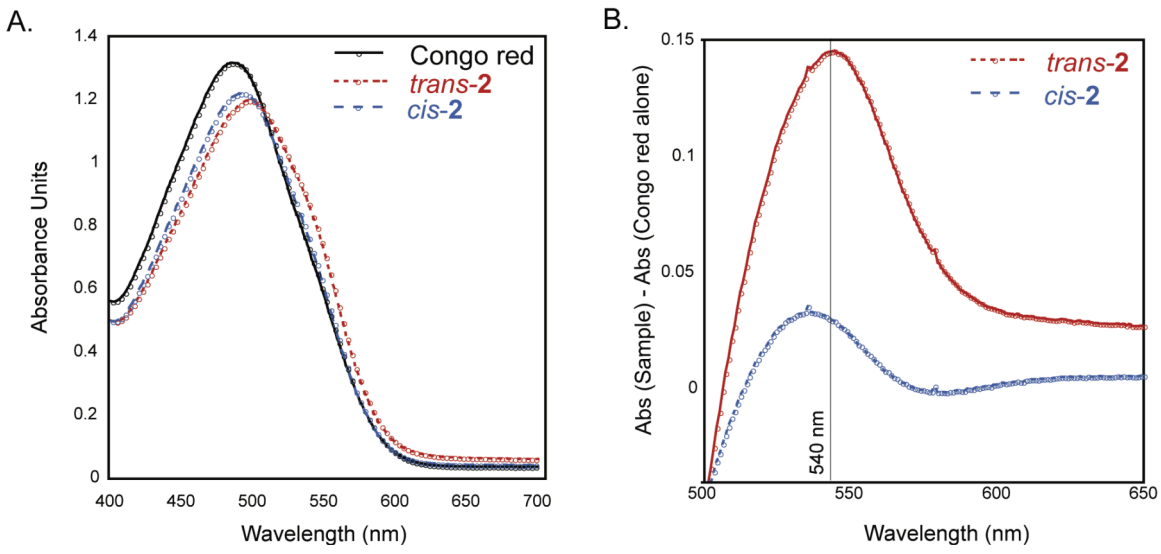

Figure S5. FT-IR spectra of photoswitched aggregates of peptide **2**. *Trans*-**2** was self-assembled into fibrils and photoirradiated to induce switching to *cis*-**2**, resulting in a coincident change in FTIR (significant loss of signal). The *cis*-**2** aggregates were then re-irradiated to *trans*-**2**, providing restoration of the characteristic β-sheet amide I stretch.

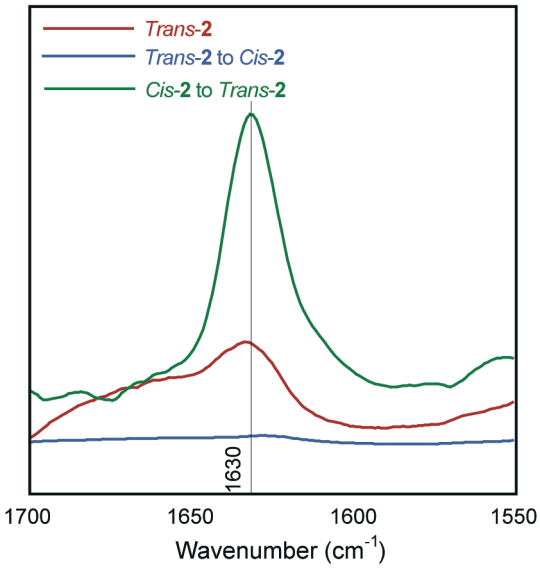

Figure S6. Analytical HPLC trace (215 nm) of Aβ42

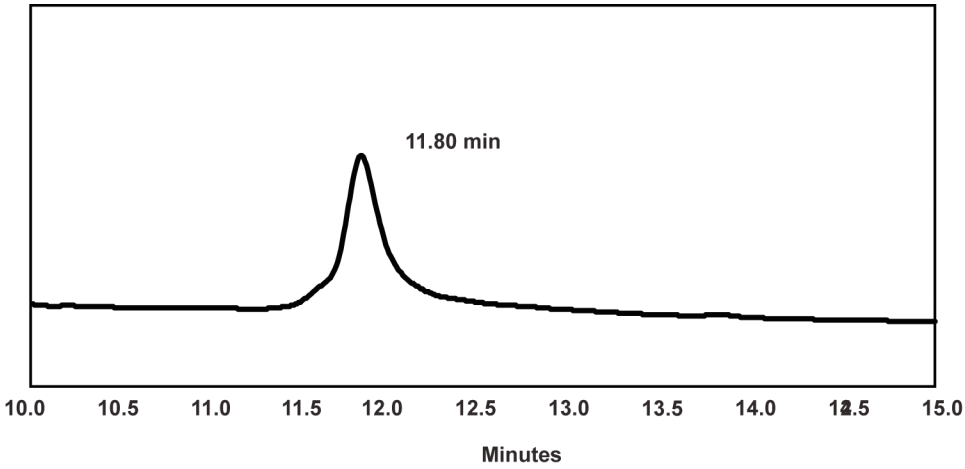

Figure S7. Analytical HPLC trace (215 nm) of *cis*-**2**

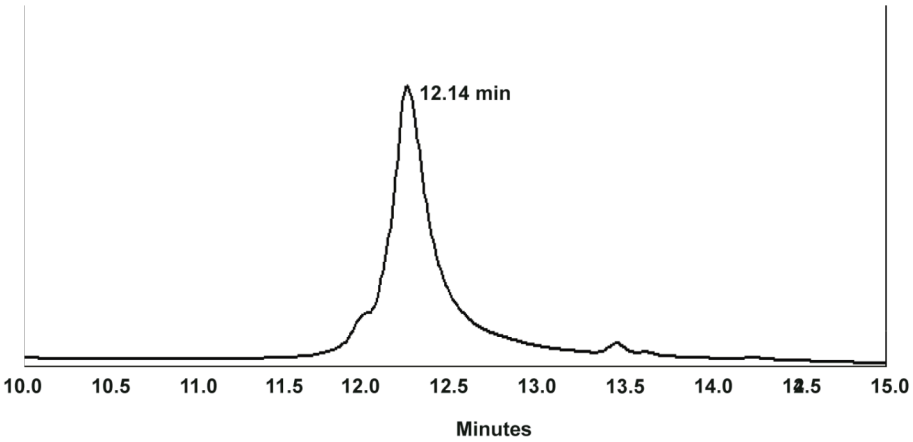

Figure S8. Analytical HPLC trace (215 nm) of *trans*-**2**

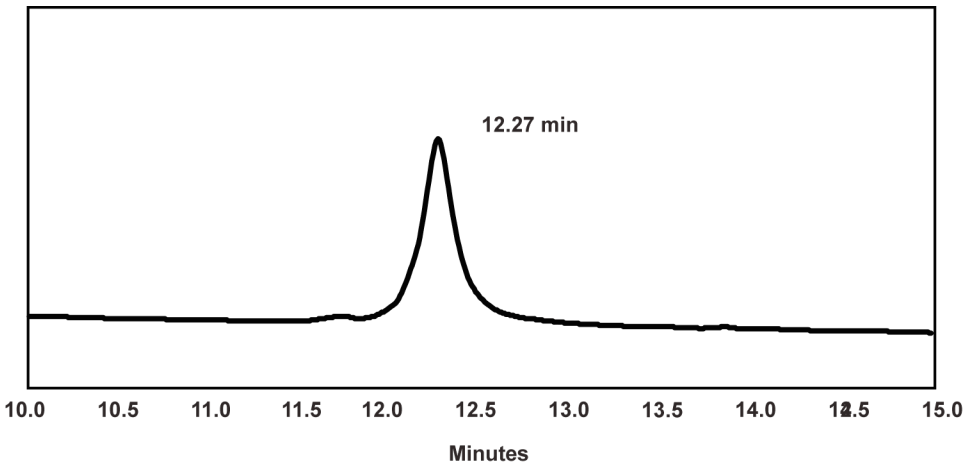

Figure S9. Analytical HPLC trace (215 nm) of *cis*-**3**

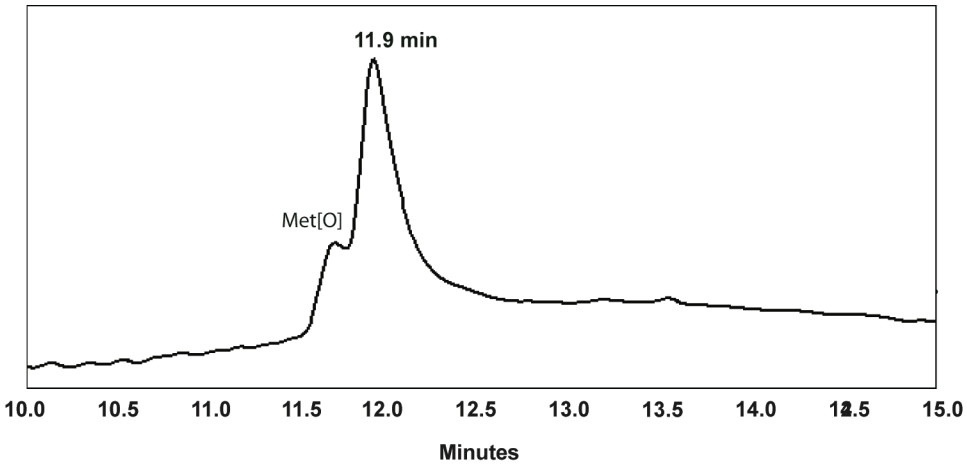

Figure S10. Analytical HPLC trace (215 nm) of *trans*-**3**

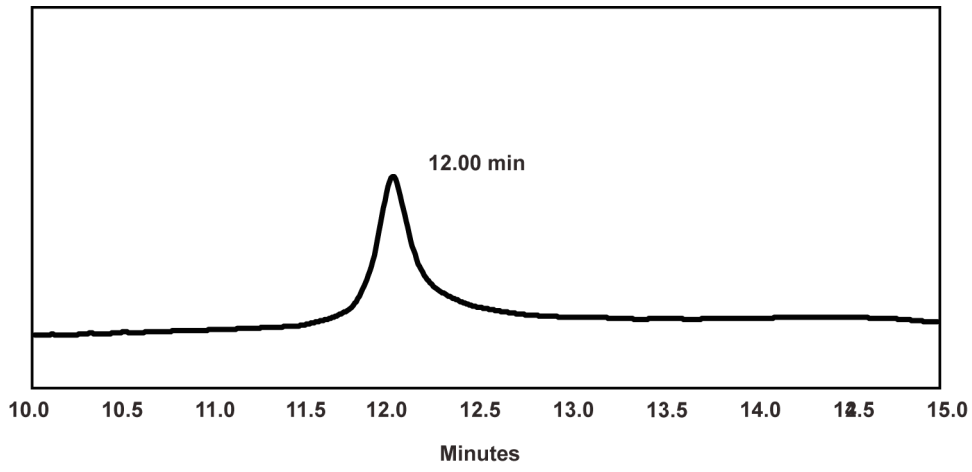

Table S1. Analytical HPLC conditions for peptides **1–3**

Peptide	**Retention time** (min)	**Gradient** (solution A: water/0.5%TFA; solution B: acetonitrile/0.5% TFA)
1	11.80	Isocratic 5% B over 5 minutes, increase 5-95% B over 15 minutes, maintain at 95% B over 5 minutes
Trans-**2**	12.27	Isocratic 5% B over 5 minutes, increase 5-95% B over 15 minutes, maintain at 95% B over 5 minutes
Cis-**2**	12.14	Isocratic 5% B over 5 minutes, increase 5-95% B over 15 minutes, maintain at 95% B over 5 minutes
Trans-**3**	12.00	Isocratic 5% B over 5 minutes, increase 5-95% B over 15 minutes, maintain at 95% B over 5 minutes
Cis-**3**	11.9	Isocratic 5% B over 5 minutes, increase 5-95% B over 15 minutes, maintain at 95% B over 5 minutes

Figure S11. MALDI-TOF mass spectrum of Aβ42

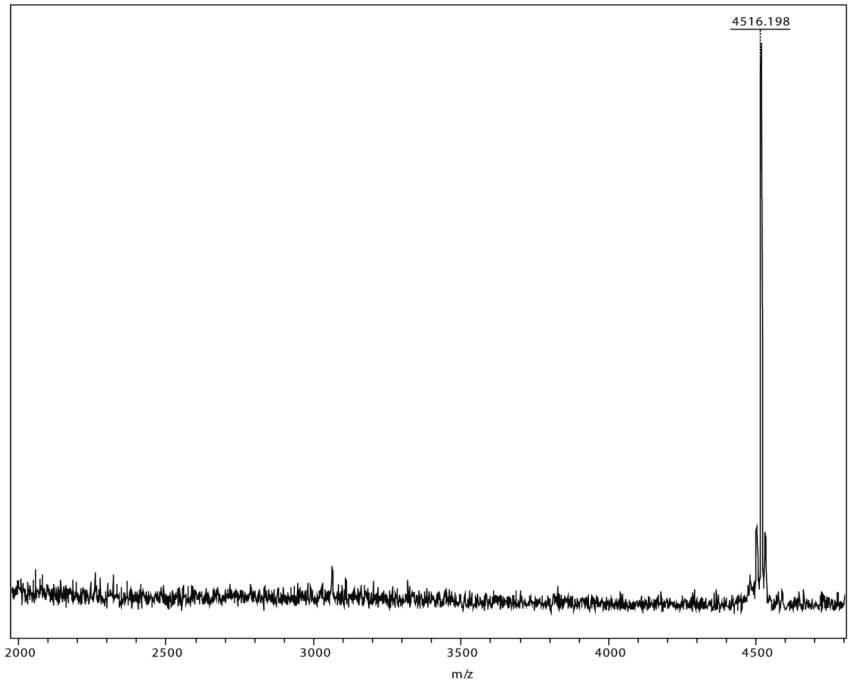

Figure S12. MALDI-TOF mass spectrum of peptide **2**.

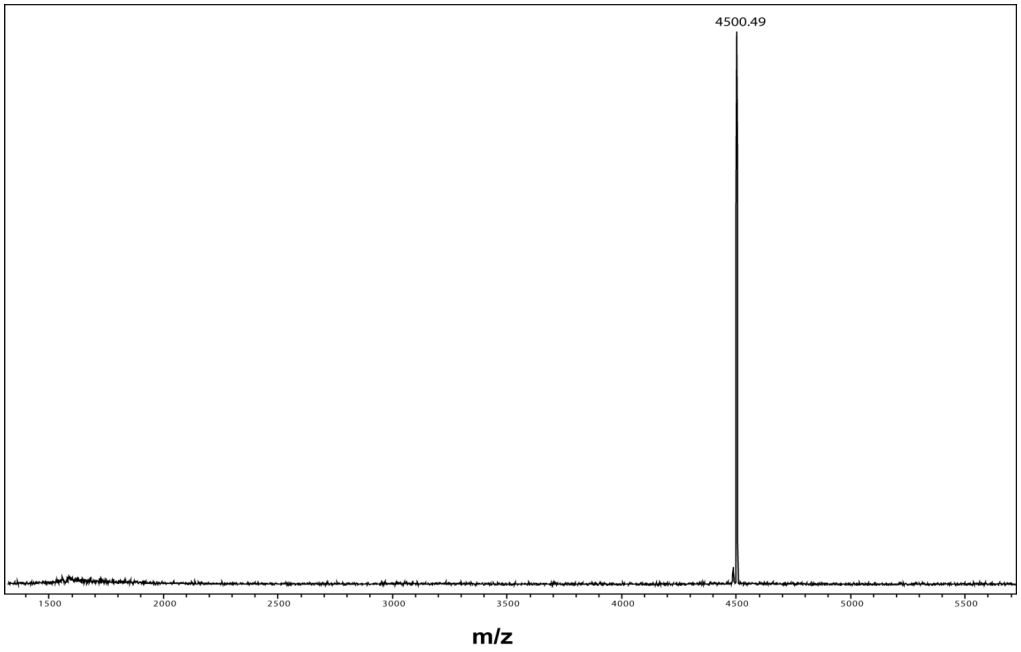

Figure S13. MALDI-TOF mass spectrum of peptide **3**

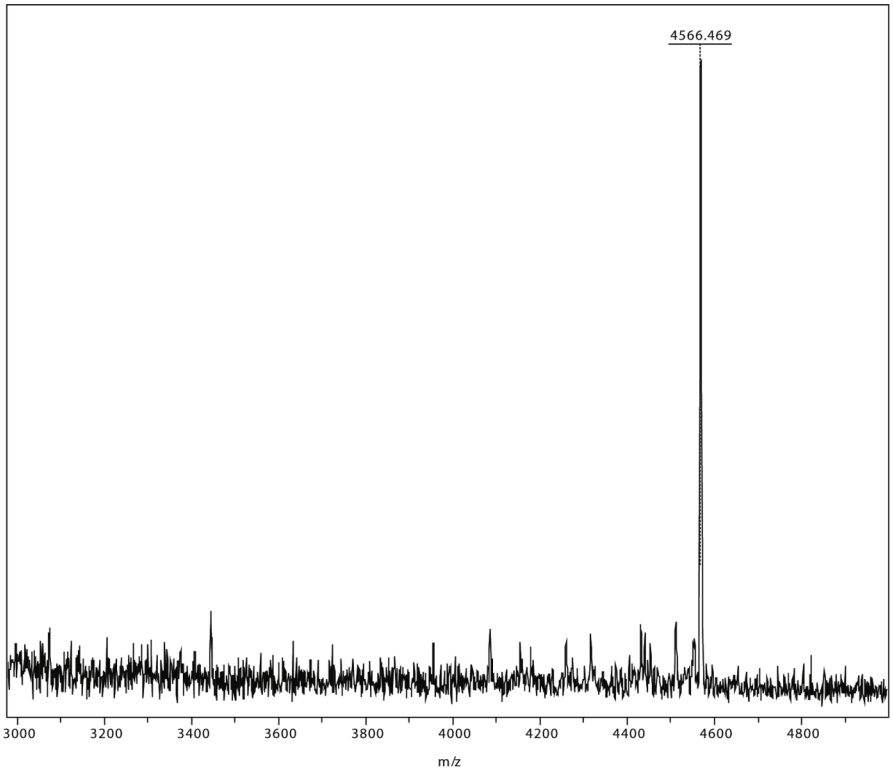

Table S1. Calculated and observed *m/z* ratios for peptides **1–3**

Peptide	Calculated m/z	Observed m/z
1	4515.0	4516.2
2	4507.0	4500.5
3	4565.1	4566.5

Figure S14. Concentration curve for peptide **1**

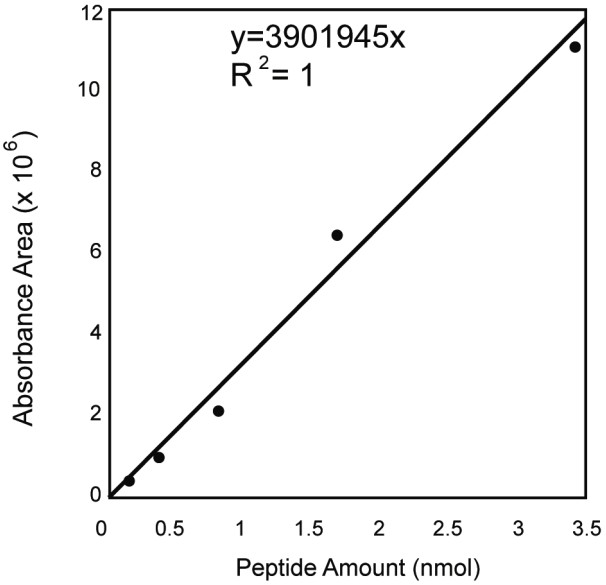

Figure S15. Concentration curve for peptides **2–3**